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EFFECTS OF SPATIAL VARIATIONS IN PACKING FRACTION ON REACTOR PHYSICS PARAMETERS IN PEBBLE-BED REACTORS

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ABSTRACT

The well-known spatial variation of packing fraction near the outer boundary of a pebble-bed reactor core is cited. The ramifications of this variation are explored with the MCNP computer code. It is found that the variation has negligible effects on the global reactor physics parameters extracted from the MCNP calculations for use in analysis by diffusion-theory codes, but for local reaction rates the effects of the variation are naturally important. Included is some preliminary work in using first-order perturbation theory for estimating the effect of the spatial variation of packing fraction on the core eigenvalue and the fission density distribution.

Key Words: Pebble-bed reactor, pebble packing, perturbation theory

1.0 INTRODUCTION

The spatial variation of void fraction (or, conversely, of packing fraction) in a cylindrical vessel filled with identical randomly packed spherical balls was studied by Benenati and Brosilow [1]. They found that the void fraction typically exhibits spatial fluctuations from a solid wall inwards for several sphere diameters before it essentially reaches an asymptotic value of approximately 39%. The details of the fluctuations depend on the ratio ***D/d*** of the vessel diameter to the sphere

diameter, but for large values of this ratio, the radial profile of void fraction is adequately represented by Figure 1.

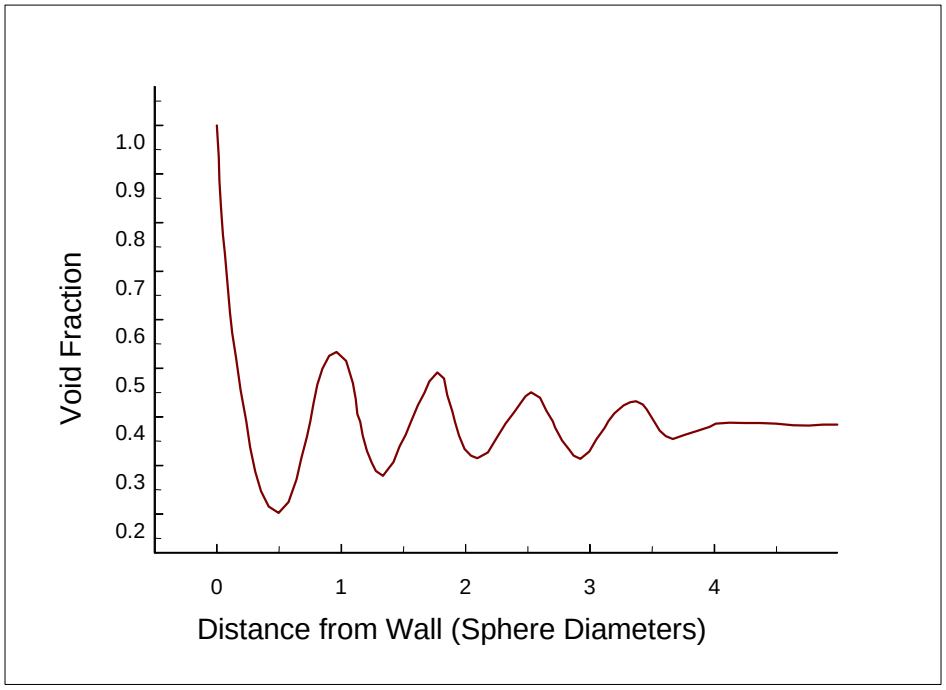

Figure 1. Variation of void fraction with distance from wall

In analyses of pebble-bed reactor (PBR) physics, it has been common (e.g., see work in Reference [2]) to neglect these spatial fluctuations and assume the packing fraction to be uniform throughout the reactor core. This would seem to be a reasonable approximation, because typical values of ***D/d*** for PBRs are of order 50. However, the volume per unit radial increment is greater near the outer edge than near the center, so the effect of a small radial band of nonuniform packing fraction near the edge may be disproportionately high, provided that the core is reflected so that the neutron flux is not relatively low there. The band of nonuniform packing near the edges should also have greater effects in a small reactor, in which the volume of that band is a greater fraction of the total core volume than it is in a larger reactor.

This paper shows that the effect on global diffusion-theory parameters is actually negligible, justifying the common practice for most purposes. However, local macroscopic cross sections differ from the average values because the atomic number density varies with the packing fraction. The paper is concluded by including some preliminary work in using first-order perturbation theory for estimating the effect of the spatial variation in the packing fraction on the core eigenvalue and the fission density distribution.

2.0 METHOD OF ANALYSIS

For a reflected PBR representing realistic design parameters, a model was constructed for the MCNP computer code [3] that comprises eleven radial zones, whose boundaries are located at the points where the curve in Figure 1 crosses the asymptotic void fraction of 39%. In each zone, the average void fraction was determined and used to find the average homogenized number densities of the constituent atomic species. Even though the edge effect also occurs at the bottom of the cylindrical vessel, the core was assumed to be axially uniform.

Another MCNP model was constructed, identical to the first except that the core composition was assumed uniform throughout. The void fraction was assumed everywhere to be 39%. This model is referred to in the following discussions as the asymptotic-density model. The composition in this model is almost, but not quite, identical to the core-averaged composition.

In the detailed model, the height was adjusted until the effective multiplication factor (k-effective) was sufficiently close to unity. Then k-effective was found for the asymptotic-density model with the same height. In both models, tallies were specified that permit the neutron flux (per source neutron), the total macroscopic cross section, the macroscopic fission cross section, and the macroscopic capture cross section to be calculated in each radial zone and for the overall reactor.

A second pair of models was constructed, in which the core comprised two regions of different fuel density. In the outer region, the fuel concentration was twice as high as in the inner region. The radial extent of the inner region was two-thirds of the core radius. The width of the outer region was deliberately chosen to be larger than the width of the annulus in which the packing fraction fluctuates, but to be small enough that the fluctuations occupied a large portion (about one-half) of the outer region. In one of these models, the radial fluctuations were modeled as in the original detailed model, and in the other, the void fraction was assumed to be 0.39 throughout.

A third detailed model was constructed, in which the diameter and the height of the core were both reduced to 1 m. It was intended to restore criticality to this core by increasing the fuel enrichment; a study with the PEBBED code [4] using a similar core showed that a fuel enrichment of about 20% would be required. This model represents a low-power reactor that has been considered for deployment in remote mining locations [5]. It was considered here because the fluctuations would occupy a much larger fraction of the core. Specific data on the various models are presented in Table I.

3.0 RESULTS

The macroscopic total, fission, and capture cross sections were determined in each radial zone and for the whole core. The macroscopic fission cross sections and the neutron fluxes are shown in Figures 2-3 for the two-region models; the results for the one-region large-core models are similar. The other cross sections behave like the fission cross section. The core-average values are shown in Table II. It can be seen that the whole-core values are remarkably close in the comparable models, even though the values in the individual zones vary substantially where the

packing fraction fluctuates. The fission cross section in the detailed model differs from asymptotic-density values by as much as 38%.

Table I. Description of MCNP Models.

Model	1-region detailed	1-region asymptotic	2-region detailed	2-region asymptotic	Small-core detailed
Core height (m)	6.32	6.32	6.32	6.32	1.0
Core diameter (m)	3.0	3.0	3.0	3.0	1.0
Reflector thickness (m)	1.0	1.0	1.0	1.0	1.0
Fuel enrichment (%)	8.0	8.0	8.0	8.0	50.0
k-effective	0.99944	0.99837	1.00309	1.00237	0.77296

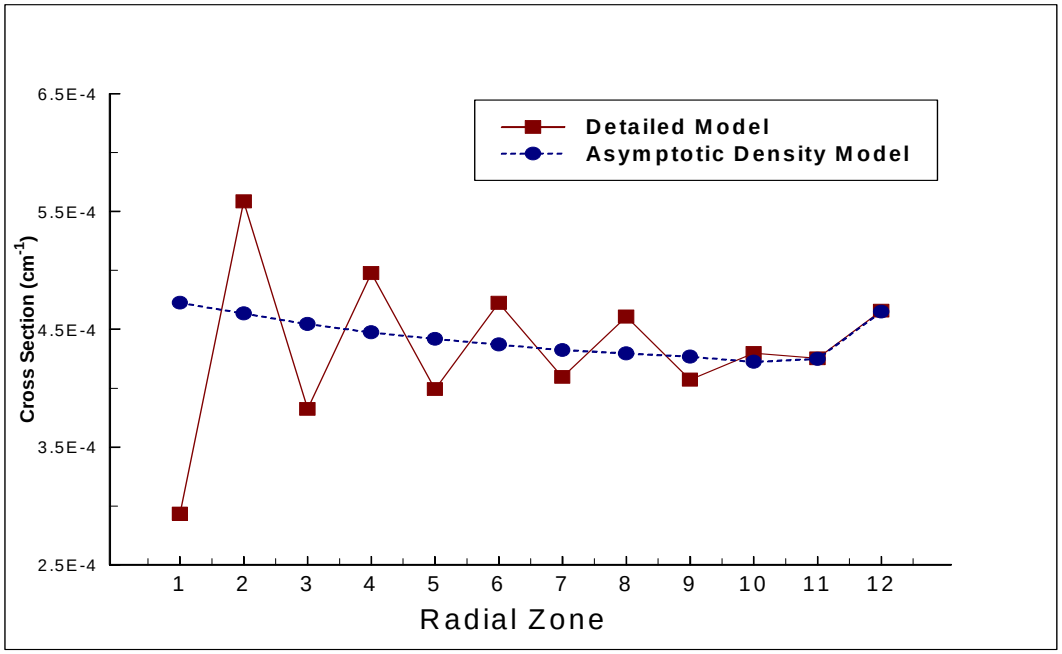

Figure 2. Macroscopic fission cross section in 2-region models.

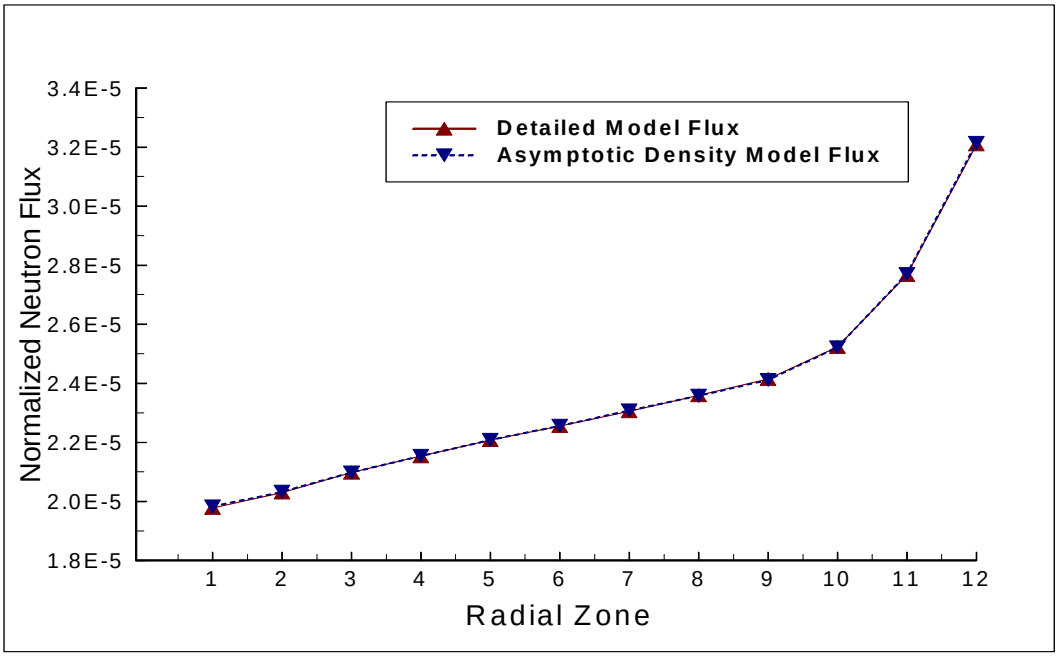

Figure 3. Neutron flux in 2-region models.

Table II. Core-average macroscopic cross sections (cm^{-1}) for various models

Model	1-region detailed	1-region asymptotic density	2-region detailed	1-region asymptotic density
Total cross section	2.6098e-1	2.6070e-1	2.6067e-1	2.6040e-1
Fission cross section	3.0996e-4	3.0946e-4	4.4997e-4	4.4903e-4
Capture cross section	2.4398e-4	2.4365e-4	2.9050e-4	2.8989e-4

The sharp upturn in the flux in the last radial zone appears because the last radial zone occupies the entire inner portion of the core, in which the spatial fluctuations in packing are no longer significant. This is a much larger zone than any of the others, and the single flux value representing the flux in this region is an average over this entire large zone.

When the enrichment was increased in the small-core model to seek a critical value, the results shown in Figure 4 were obtained. For the fuel pebble design on which these analyses were based (a design similar in dimensions, microsphere density, and microsphere design to typical PBR power plant designs), it is not possible to achieve criticality in this small core by increasing the

enrichment – that is, according to this MCNP model. However, the PEBBED model of a similar reactor did achieve criticality at an enrichment of about 20%. The difference in the results is due to the treatment of the heterogeneity of the actual reactor. PEBBED accounts for the double heterogeneity in the PBR by appropriate Dancoff factors, but the MCNP model applies no such correction. In references [5] and [6] MCNP models are described that explicitly represent one or two levels of heterogeneity: one level models each individual pebble, and two levels represent each individual microsphere in each pebble. This fine detail is achieved by using the repeating structures feature of MCNP, so that it is only necessary to model the basic cell on each level. However, this approach requires that the microspheres or pebbles be modeled as though they were arranged in a regular lattice, whereas in reality they are packed randomly. Because the fluctuations in packing fraction near the walls of a PBR occur on a length scale comparable to a pebble radius, it is not even practical to represent these fluctuations in an MCNP model by such techniques as varying the distance between lattice points (i.e., artificially not allowing the pebbles to touch). It does not seem practical to use MCNP to model such small cores at all.

For larger cores, it is understood that representing the core or regions of it as homogeneous in MCNP models leads to inaccuracies in the numerical values of the calculation results. However, when, as in this paper, the results are only used to show trends or relative values, the exact numerical values are unimportant, and the conclusions drawn from such calculations remain valid.

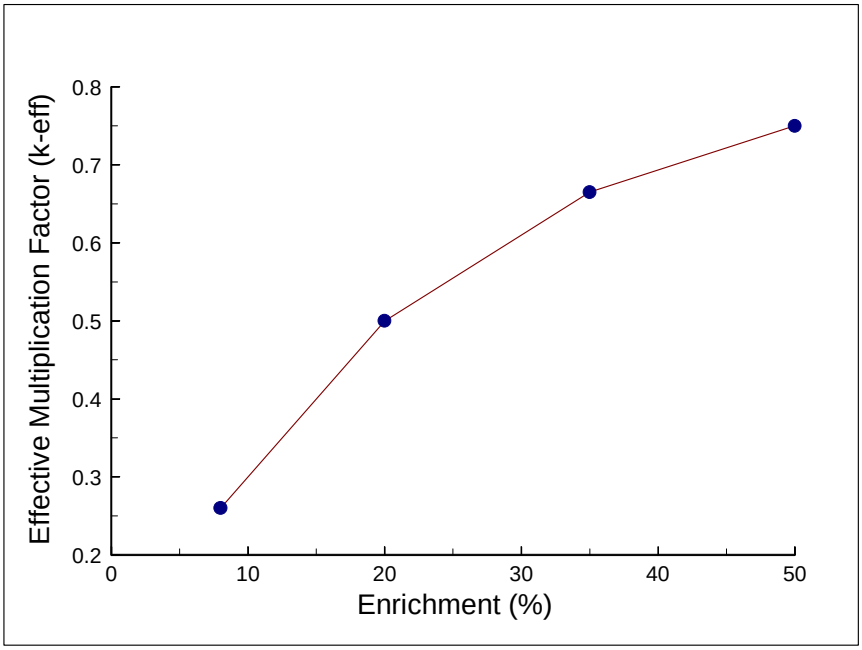

Figure 4. k-effective vs. fuel enrichment for small reactor core.

4.0 DISCUSSION

The results of this study vindicate the standard practice of assuming the packing fraction to be uniform across the diameter of a pebble-bed reactor whose radial extent is many pebble diameters, if the issues of interest are restricted to global phenomena and parameters. However, if local reaction rates are important, then the radial fluctuations in packing fraction near the outer perimeter should be taken into account.

5.0 ON THE USE OF PERTURBATION THEORY

The spatial variation in the fuel pebble packing fraction translates into a corresponding variation in the fuel atom density or equivalently the macroscopic cross sections. This variation directly affects the power distribution in the core. In this section we report work in progress on the application of perturbation theory to the packing fraction variation problem and discuss its validity and challenges. In particular we report a preliminary development of formalisms for the change in the solution (eigenvalue and normalized fission density distribution) caused by the variation in the packing fraction (fuel density ρ_{fuel}) from the nominal (average) value; i.e.,

$$\rho_{\text{fuel}} = \rho_{\text{ave}} + \varepsilon\rho_1(\underline{r}) \tag{1}$$

In terms of the atom density, Eq. (1) is equivalent to

$$n_{fuel} = n_o + \varepsilon\, n_1(\underline{r}) = n_o(\underline{r})(1+\varepsilon n_1(\underline{r})/n_o) \equiv n_o(\underline{r})(1+\varepsilon N(\underline{r})) \tag{2}$$

In Eqs. (1) and (2), n_o and ρ_{ave} are the average atom and fuel densities, respectively. $N_1(\underline{r})$ or $\rho_1(\underline{r})$ are the deviations in the corresponding average quantities as functions of position from the wall and N is the ratio of the change in the atom density to the average value. Since a change in ρ or n can be modeled as a change in the macroscopic cross sections (diffusion operators H & F), we define the unperturbed problem as the case with the average packing fraction:

$$\begin{cases} H_o\phi_o = \lambda_o F_o\phi_o \text{ in V} \\ B\phi_o = 0 \text{ on } \partial V \end{cases} \tag{3}$$

In the above equations, F_o and H_o are the one-group fission and diffusion operators defined in the volume V. They are given as in Eqs. (5) below with the cross sections (diffusion constants) subscripted with "o." The operator B is the homogeneous boundary condition operator to be defined when needed. The external surface bounding V is designated as ∂V. If the cross sections (atom densities) are perturbed according to Eq. (2), then the perturbed system is defined as

$$\begin{cases} H\ \phi = \lambda\ F\ \phi \text{ in V} \\ B\ \phi = 0 \text{ on } \partial V \end{cases} \tag{4}$$

where

$$\begin{cases} \boldsymbol{H}\phi \equiv -\underline{\nabla}\cdot\boldsymbol{D}(\underline{\boldsymbol{r}})\underline{\nabla}\phi(\underline{\boldsymbol{r}}) + \Sigma_{\boldsymbol{a}}(\underline{\boldsymbol{r}})\phi \\ \boldsymbol{F}\phi \equiv \Sigma_{\boldsymbol{f}}(\underline{\boldsymbol{r}})\phi(\underline{\boldsymbol{r}}) \end{cases} \tag{5}$$

with

$$\begin{cases} \boldsymbol{D}(\underline{\boldsymbol{r}}) \equiv \boldsymbol{D_o}(\underline{\boldsymbol{r}})\{1-\varepsilon\boldsymbol{N}(\underline{\boldsymbol{r}})/(1+\varepsilon\boldsymbol{N}(\underline{\boldsymbol{r}}))\} \\ \Sigma_{\boldsymbol{x}}(\underline{\boldsymbol{r}}) \equiv \Sigma_{\boldsymbol{x}}(\underline{\boldsymbol{r}})(1+\varepsilon\boldsymbol{N}(\underline{\boldsymbol{r}})), \quad \boldsymbol{x} = \text{reaction type} \end{cases} \tag{6}$$

Use the subscript "$\boldsymbol{o}$" on all the cross sections and the flux in Eq. (5) to get the equations for $\boldsymbol{H_o\phi_o}$ and $\boldsymbol{F_o\phi_o}$. The parameter of interest in this work is the fission (power) distribution defined as

$$\boldsymbol{P}(\underline{\boldsymbol{r}}) = \frac{\int_{\mathrm{v}} \boldsymbol{dV}\, \boldsymbol{f}(\underline{\boldsymbol{r}},\underline{\boldsymbol{r}_o})\phi(\underline{\boldsymbol{r}})}{\int_{\mathrm{v}} \boldsymbol{dV}\, \phi(\underline{\boldsymbol{r}})} \quad , \tag{7}$$

where

$$\boldsymbol{f} \equiv \Sigma_{\boldsymbol{f}}(\underline{\boldsymbol{r}})\ \delta(\underline{\boldsymbol{r}} - \underline{\boldsymbol{r}_o}) \equiv \mathrm{N}(\underline{\boldsymbol{r}})\sigma_{\boldsymbol{f}}(\underline{\boldsymbol{r}})\ \delta(\underline{\boldsymbol{r}} - \underline{\boldsymbol{r}_o}) \tag{8}$$

In Eq. (7), $\boldsymbol{P}(\underline{\boldsymbol{r}})$ is the normalized fission distribution. It is assumed that the microscopic cross section $\sigma_{\boldsymbol{f}}(\underline{\boldsymbol{r}})$ is not perturbed.

We follow standard perturbation theory and proceed to obtain an expression for $\boldsymbol{P}$ in terms of the unperturbed quantity. Assume

$$\phi = \phi_{\boldsymbol{o}} + \varepsilon\ \phi_1 + .. \tag{9}$$

$$\boldsymbol{P} = \boldsymbol{P_o} + \varepsilon\ \boldsymbol{P}_1 + ... \tag{10}$$

Define

$$\langle a,b \rangle = \int_{\mathrm{v}} \boldsymbol{d}\mathrm{v}\ a\ b \tag{11}$$

Then Eq. (7) can be written as

$$\boldsymbol{P}\ \langle\phi\rangle = \langle \boldsymbol{f}(\underline{\boldsymbol{r}},\underline{\boldsymbol{r}_o}),\ \phi(\underline{\boldsymbol{r}})\rangle_{\underline{\boldsymbol{r}}} \tag{12}$$

In the above equation, the subscript $\boldsymbol{r}$ on the right bracket implies integration over the $\underline{\boldsymbol{r}}$ volume. Substitution of Eqs. (2) and (9) in Eq. (12) gives

$$\begin{aligned} &\boldsymbol{P_o}<\phi_o> + \varepsilon\, \boldsymbol{P_o}<\phi_1> + \varepsilon \boldsymbol{P}_1<\phi_0> \\ &= <\boldsymbol{N_o}\sigma_f + \varepsilon\, \boldsymbol{N}_1\, \sigma_f,\, \phi_o + \varepsilon\, \phi_1> \\ &= <\boldsymbol{N_o}\sigma_f \delta_1\phi_o> + \varepsilon<\boldsymbol{N_o}\sigma_f \delta_1\phi_1> + \varepsilon<\boldsymbol{N}_1\sigma_f \delta_1\phi_o> \end{aligned} \tag{13}$$

Equating the first-order terms in Eq. (13) yields

$$\boldsymbol{P}_1(\underline{\boldsymbol{r}}_o)<\phi_o>=\boldsymbol{N}_1(\underline{\boldsymbol{r}}_o)\sigma_f(\underline{\boldsymbol{r}}_o)\phi_o(\underline{\boldsymbol{r}}_o)+ <\boldsymbol{g}(\underline{\boldsymbol{r}},\underline{\boldsymbol{r}}_o),\, \phi_1(\underline{\boldsymbol{r}})>_{\underline{\boldsymbol{r}}} \tag{14}$$

where

$$\begin{aligned} \boldsymbol{g}(\underline{\boldsymbol{r}},\underline{\boldsymbol{r}}_o) &\equiv \boldsymbol{N_o}(\underline{\boldsymbol{r}})\sigma_f(\underline{\boldsymbol{r}})\, \delta(\underline{\boldsymbol{r}}-\underline{\boldsymbol{r}}_o) - \boldsymbol{P_o}(\underline{\boldsymbol{r}}_o) \\ &= \Sigma_{f\boldsymbol{o}}(\underline{\boldsymbol{r}})\, \delta(\underline{\boldsymbol{r}},\underline{\boldsymbol{r}}_o) = \boldsymbol{P_o}(\underline{\boldsymbol{r}}_o) \end{aligned} \tag{15}$$

To determine $\boldsymbol{P}_1$, one must find the last term on the right-hand side (RHS) of Eq. (14), which is the only unknown term. This can be done by finding the governing equation for φ_1. Substitute Eq. (5) in Eq. (4) and equate the first order terms to get the equation satisfied by φ_1:

$$(\boldsymbol{H_o}-\lambda_o\boldsymbol{F_o})\phi_1 = -(\boldsymbol{H}_1-\lambda_o\boldsymbol{F}_1)\phi_o + \lambda_1\boldsymbol{F_o}\phi_o \tag{16}$$

Since the boundary condition is not perturbed, it can be shown that

$$\boldsymbol{B}\,\phi_1 = 0 \text{ on } \partial\boldsymbol{V} \tag{17}$$

Taking the inner product of Eq. (16) with an adjoint function to be define shortly yields

$$<\varphi_o^*,(\boldsymbol{H_o}-\lambda_o\,\boldsymbol{F_o})\phi_1> = -<\varphi_o^*,(\boldsymbol{H}_1-\lambda_o\,\boldsymbol{F}_1)\phi_o>+ \lambda_1<\varphi_o^*,\, \boldsymbol{F_o}\phi_o> \tag{18}$$

Since the boundary condition is not perturbed, then

$$<\phi_1,\left(\boldsymbol{H}_o^*-\lambda_o\,\boldsymbol{F}_o^*\right)\phi_o^*>= -<\phi_o^*,(\boldsymbol{H}_1-\lambda_o\,\boldsymbol{F}_1)\phi_o>+ \lambda_1<\varphi_o^*,\, \boldsymbol{F_o}\phi_o> \tag{19}$$

To simplify Eq. (19), we choose

$$\begin{cases} (\boldsymbol{H_o}-\lambda_o\boldsymbol{F_o})\phi_o^*(\underline{\boldsymbol{r}}) = \boldsymbol{g}(\underline{\boldsymbol{r}},\underline{\boldsymbol{r}}_o) \text{ in } \boldsymbol{V} \\ \boldsymbol{B}\,\phi_o^* = 0 \text{ on } \partial\boldsymbol{V} \end{cases} \tag{20}$$

Then, Eq. (20) becomes

$$<\phi(\underline{\boldsymbol{r}},\boldsymbol{E}),\, \boldsymbol{g}(\underline{\boldsymbol{r}},\underline{\boldsymbol{r}}_o,\boldsymbol{E})>_{\underline{\boldsymbol{r}}}= -<\phi_o^*(\boldsymbol{H}_1-\lambda_o\,\boldsymbol{F}_1)\phi_o> + \lambda_1<\phi_o^*,\, \boldsymbol{F_o}\,\phi_o> \tag{21}$$

In order for the solution to Eq. (20) to exist, the Fredholm alternative requires that

$$<\phi_o(\underline{r}) \ , \ g(\underline{r},\underline{r}_o)>_{\underline{r}} \ = 0 \tag{22}$$

Further, the solution to Eq. (21) is not unique. To simplify Eq. (19), we choose the uniqueness condition to be

$$<\phi_o^* \ , \ F_o\phi_o> \ = 0 \tag{23}$$

We note that Eq. (20) always has a solution since Eq. (22) is satisfied because of the definition in Eq. (15). Now the substitution of Eq. (21) into Eq. (14) yields the final result for the change in the fission density.

$$P_1(\underline{r}_o) \int_v dV \ \phi_o(\underline{r}) = N_1(\underline{r}_o) \ \sigma_f(\underline{r}_o)\phi_o(\underline{r}_o) + \int_v dV \phi_o^*(\underline{r},\underline{r}_o)(H_1 - \lambda_o F_1)\phi_o(\underline{r}) \tag{24}$$

The expression for the change in the eigenvalue can be found in many papers and texts. Consistent with the notation in this paper, we have

$$\lambda_1 = \frac{<\varphi_o^*, (H_1 - \lambda_o F_1)\phi_o>}{<\varphi_o^*, F_o\phi_o>} \tag{25}$$

where φ_o^* is the standard adjoint solution given to

$$(H_o - \lambda_o F_o)\varphi_o^* = 0 \text{ in } V \tag{26}$$

$$B\varphi_o^* = 0 \text{ on } \partial V \tag{27}$$

The verification of the correctness of these expressions (24 and 25) for the PBR problem with packing fraction variation is in progress. We note that the perturbation development in this paper is not new except for its application to the packing fraction variation in PBRs and the expression for power (fission) density distribution.

Two challenges are worth pointing out. First, it is seen from Figure 1 that the perturbation from the average packing is large (i.e., not first order) and therefore first-order perturbation theory may not yield results with desired accuracy. For example, in the first wave from the wall, the change in the cross section from the average value is almost a factor of 2. We expect to consider high-order perturbation theory to overcome this problem.

As further seen from Figure 1, the void fraction approaches unity near the core wall. In this case, diffusion theory is no longer valid and as a result one must resort to perturbation analysis in transport theory. This problem may be approximated by representing the wiggles in the packing fraction as smeared step functions. A sample calculation shows the potential for this approach.

Consider a slab geometry in which the only perturbation is in the diffusion coefficient, which changes from D_l to D_r at $x=x'$. Eq. (25) can be recast into the form

$$\lambda_1 = -\frac{1}{\left\langle \bar{\varphi}_0^* \boldsymbol{F}_0 \bar{\varphi}_0 \right\rangle}\left[\left\langle \bar{\varphi}_0^*, \boldsymbol{D}_1(\boldsymbol{x})\bar{\varphi}_0'' \right\rangle + \bar{\varphi}_0^*(\boldsymbol{x}')\nabla\bar{\varphi}_0(\boldsymbol{x}')(\boldsymbol{D}_r - \boldsymbol{D}_l)\right], \tag{28}$$

where the overbar on the flux indicates a normalization such that the phase space integral is equal to unity.

In a one-group formulation, the following parameters are chosen for numerical evaluation:

$D_0 = 0.5$
$D_1 = -0.1,\ x<0.5$
$D_1 = 0.1,\ x>0.5$
$\Sigma_a = 1.0$
$\nu\Sigma_f = 2.0.$

The current is set equal to zero at $x=0$ and the flux is set equal to zero at $x=1$.

This problem can also be solved "exactly" by computer. Table III shows the eigenvalues for the unperturbed, first-order, and exact cases, and Figure 5 shows the fluxes (the first-order flux is obtained from Eq. (24) and the definition of the fission density).

Table III. Eigenvalues in Unperturbed, First-Order, and Exact Cases

Order	Eigenvalue	Error %
0^{th} (Unperturbed)	1.117	-9%
1^{st}	1.039	-1%
Exact	1.025	0%

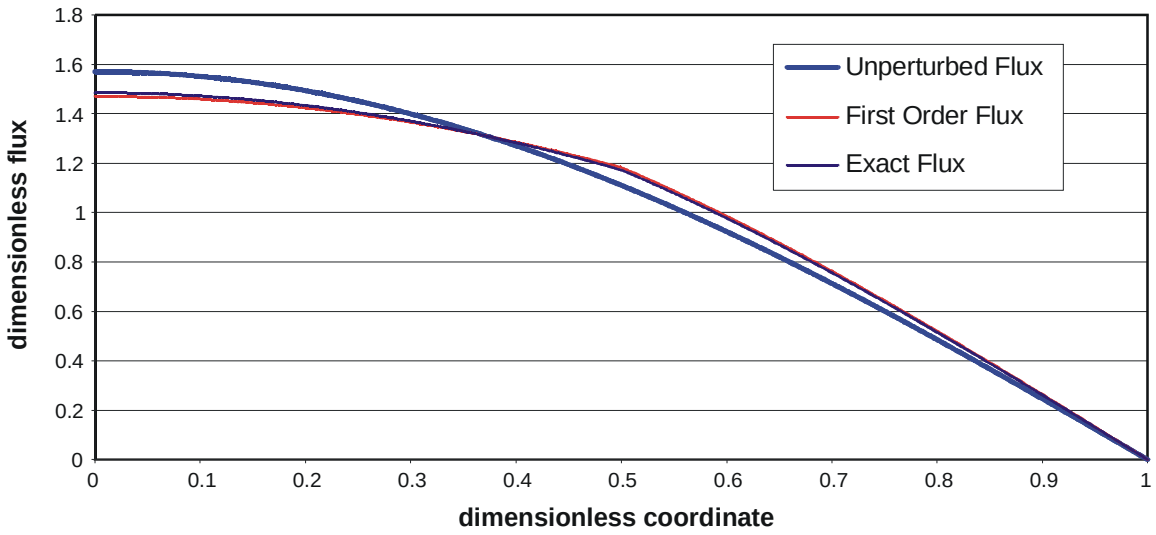

Figure 5. One-group Fluxes in Unperturbed, First-order, and Exact Cases

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